Supernodes ordering to enhance Block Low-Rank compression in sparse direct solvers

Grégoire Pichon, Eric Darve, Mathieu Faverge, Pierre Ramet, Jean Roman

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Context

PaStiX library

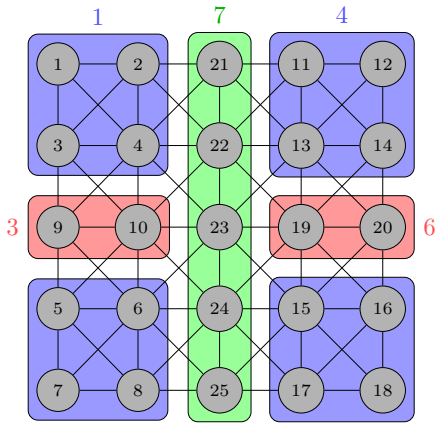
- Sparse direct solver with supernodal method
- Right-looking scheduling strategy
- Block low-rank support:
  - Large blocks are compressed into a low-rank form
  - Similar global behavior to the full-rank solver
  - *Minimal Memory* strategy to save memory
  - *Just-In-Time* strategy to reduce time-to-solution

Objective of this talk: study low-rank clustering strategies to enhance blocks compressibility

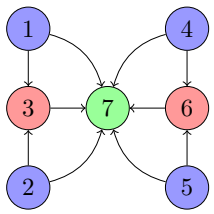
Symbolic Factorization

General approach

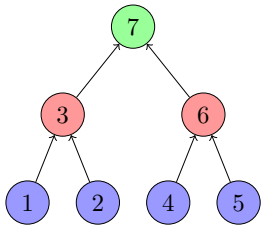
1. Build a partition with the nested dissection process
2. Compress information on data blocks
3. Compute the block elimination tree using the block quotient graph



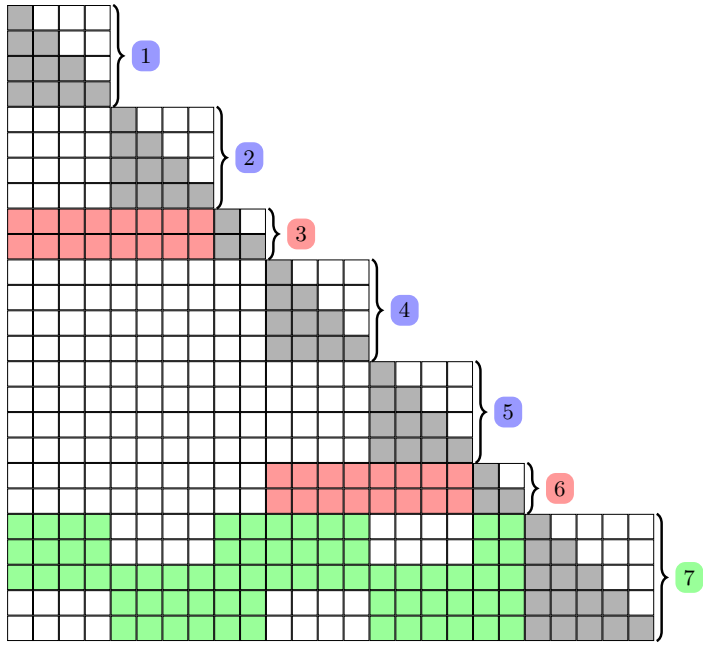
Adjacency graph (G).



Quotient graph (G^*/P) $= (G/P)^*$

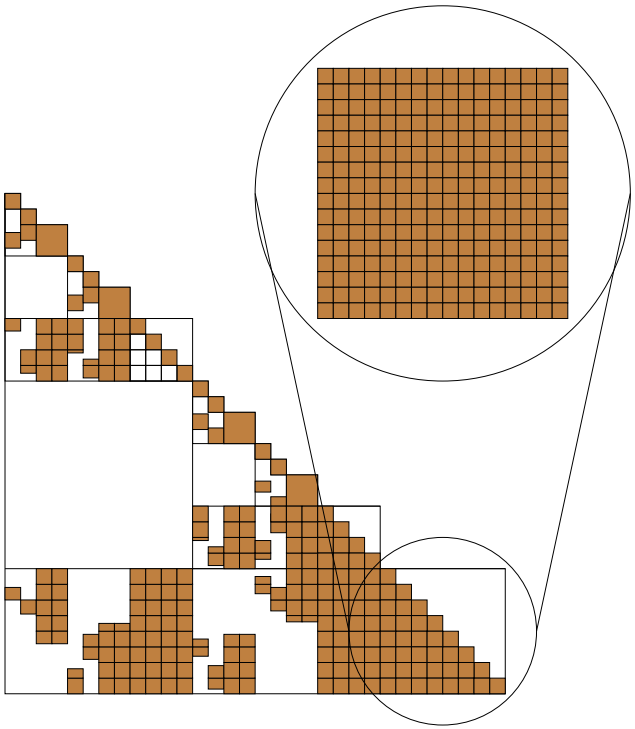


Elimination tree (T).



Factorized matrix (L).

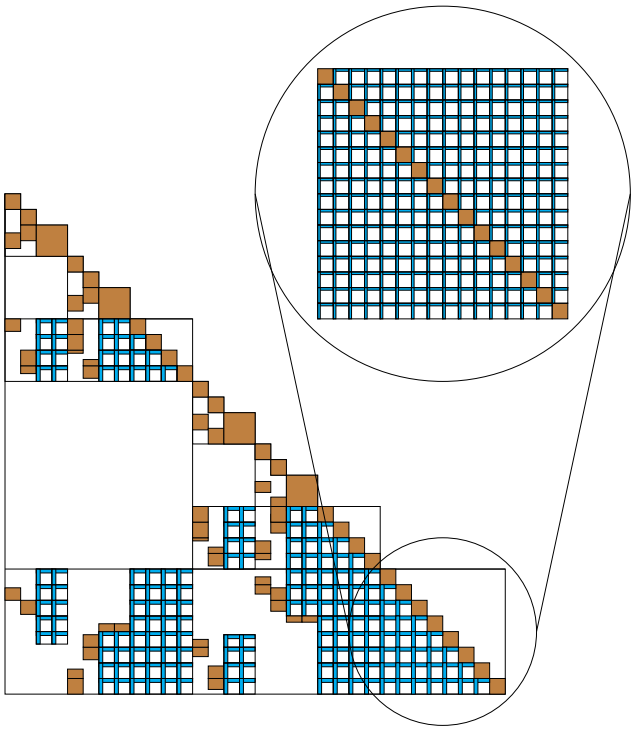
From full-rank to low-rank



Full-rank algorithm

- For each column-block / supernode:
  1. **Factorize** the diagonal block (POTRF/GETRF)
  2. **Solve** off-diagonal blocks in the current column (TRSM)
  3. **Update** the trailing matrix (GEMM)

From full-rank to low-rank

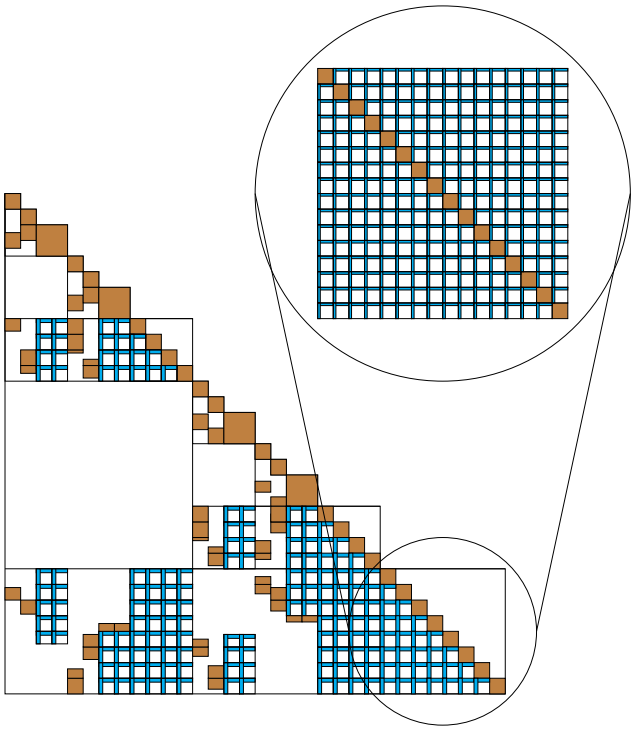


Just-In-Time algorithm

- For each column-block / supernode:
  1. **Factorize** the diagonal block (POTRF/GETRF)
  2. **Compress** off-diagonal blocks
  3. **Solve** low-rank off-diagonal blocks in the current column (TRSM)
  4. **Update** the trailing matrix (LR2FR)

- Reduce the time to solution
- Memory peak is as large as full-rank

From full-rank to low-rank

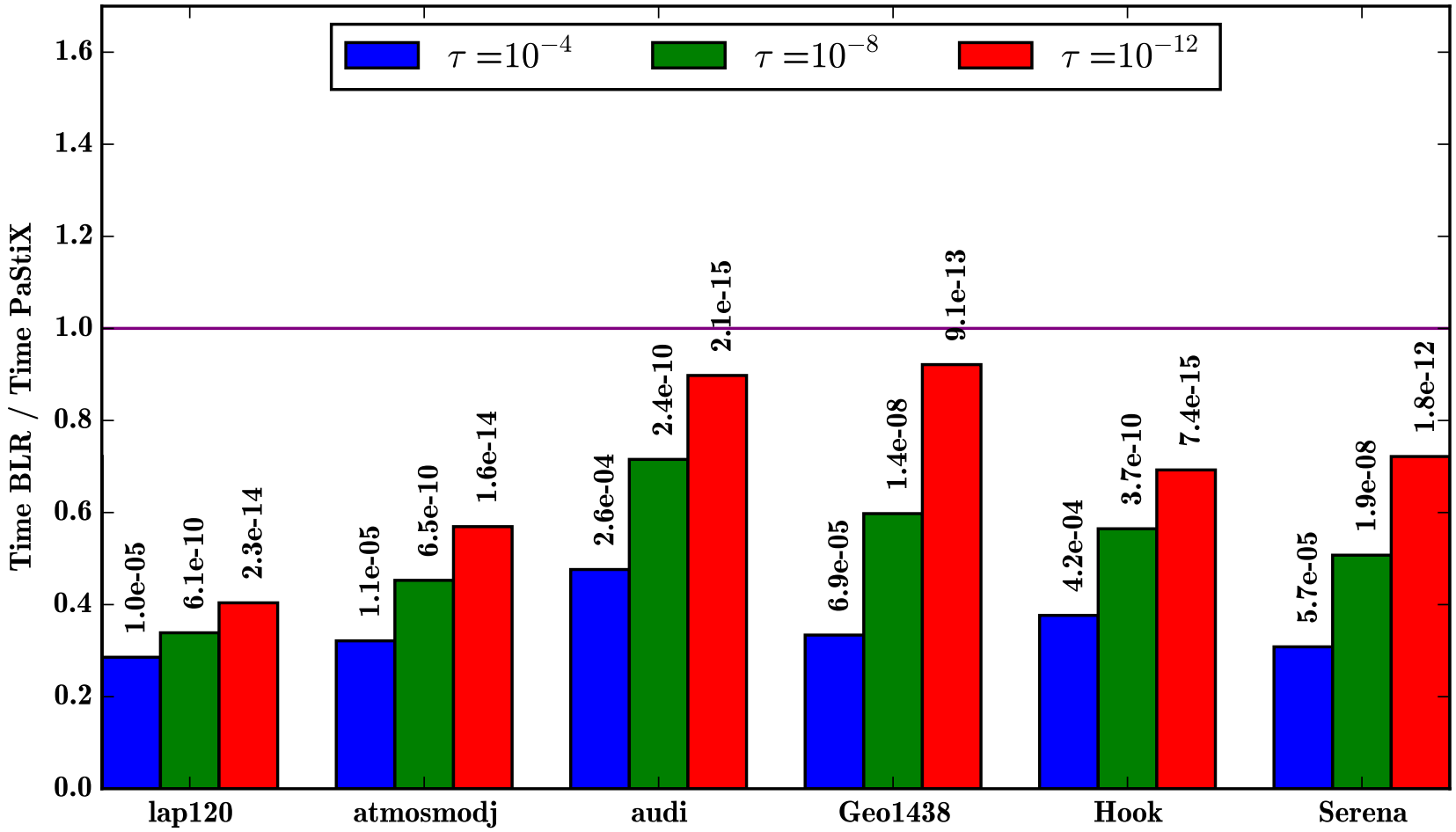


Minimal Memory algorithm

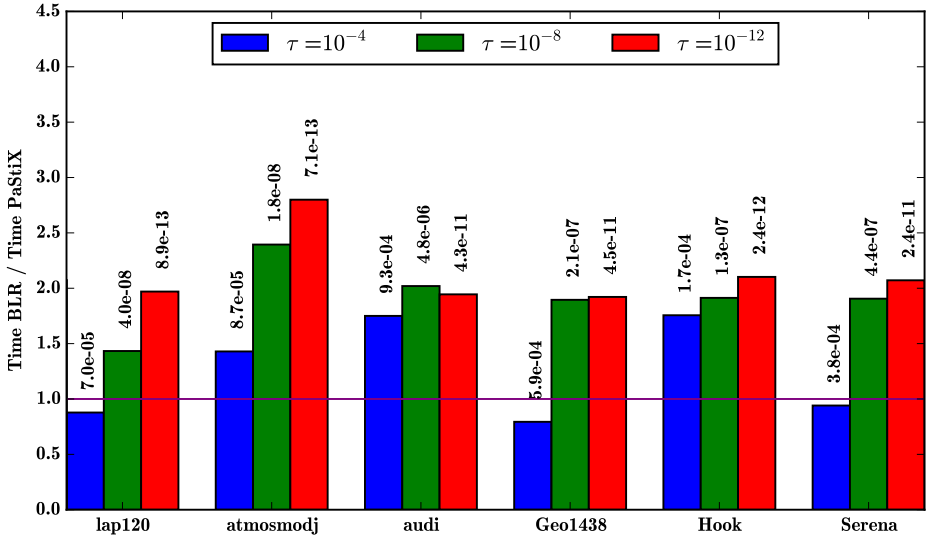
- Compress all off-diagonal blocks
- For each column-block / supernode:
  1. **Factorize** the diagonal block (POTRF/GETRF)
  2. **Solve** low-rank off-diagonal blocks in the current column (TRSM)
  3. **Update** the trailing matrix (LR2LR)

- Reduce the memory peak of the solver
- LR2LR updates may be too costly for *small* cases

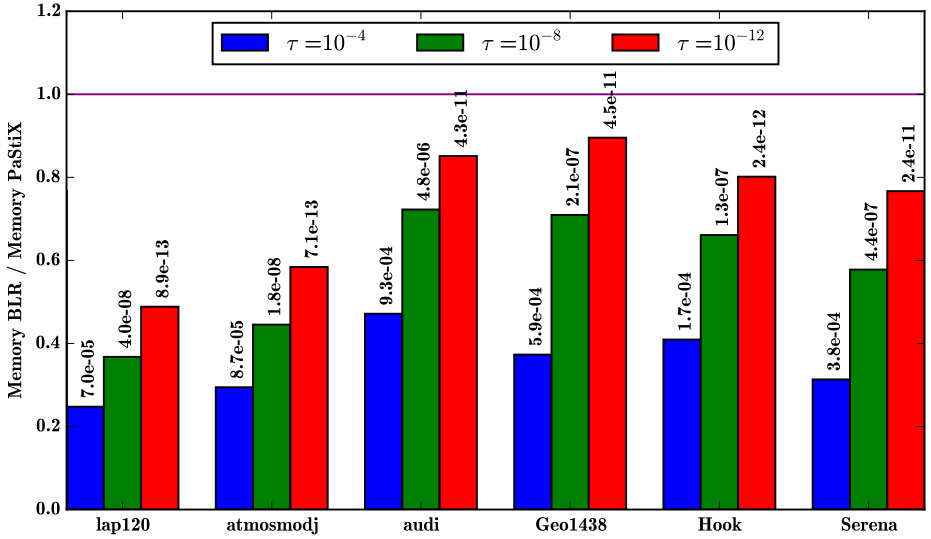
Performance of RRQR/*Just-In-Time*



Performance of RRQR/*Minimal Memory*

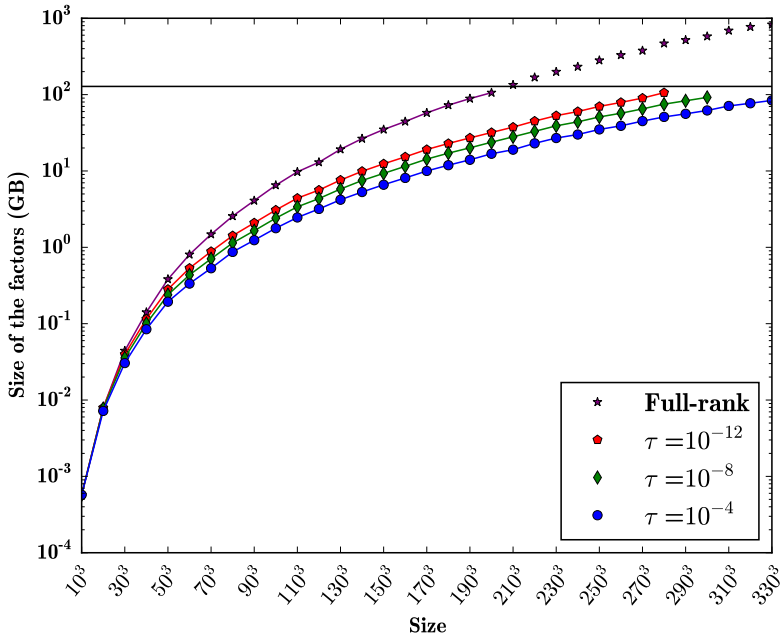


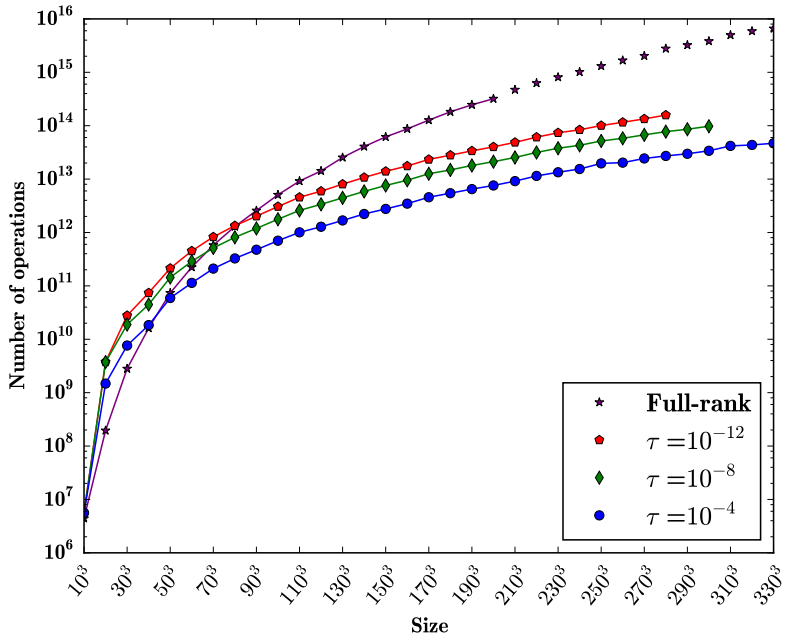
Factorization time



Memory footprint

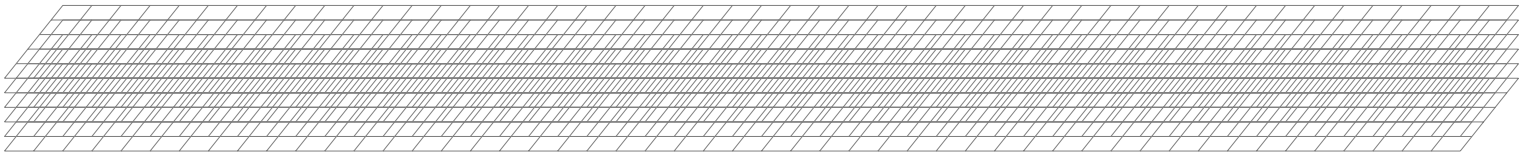
Scalability of *Minimal Memory* strategy on Laplacian matrices





- $128GB$ of memory
- Up to $8M$ unknowns in full-rank
- Up to $36M$ unknowns with $\tau = 10^{-4}$

Up to what limit?

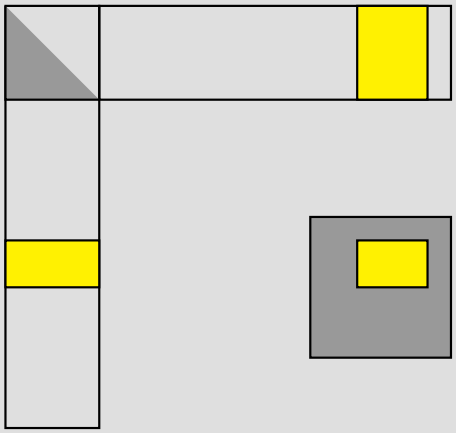


- 96 cores machine with 3TB of memory
- $100 \times 100 \times 100K$ mesh
- Full-rank would have required $11TB$ of memory
- With $\tau = 10^{-4}$:
  - Only $2TB$ of memory for the coefficients
  - Less than 6 hours to factorize
  - 10^{-8} solution with 15 iterations of iterative refinement

Summary of the updates

Cost of applying a $m \times n$ update to a $M \times N$ block.

Full rank



- A single GEMM kernel
- Cost depends on mn

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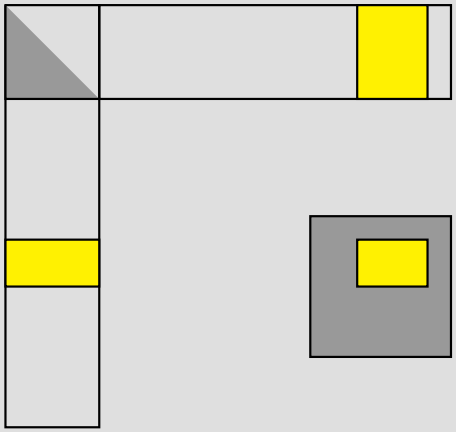

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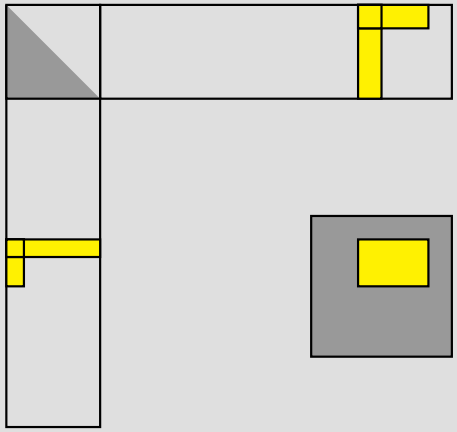
Just-In-Time



- Serie of small GEMM kernels
- Cost depends on mn

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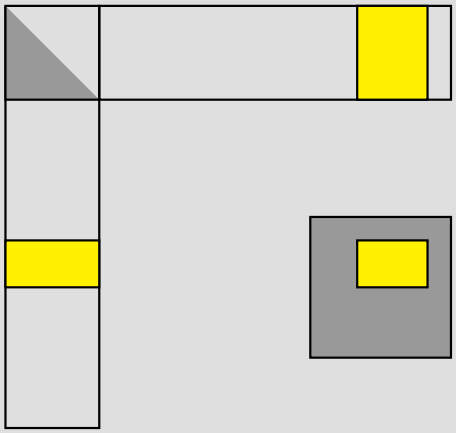

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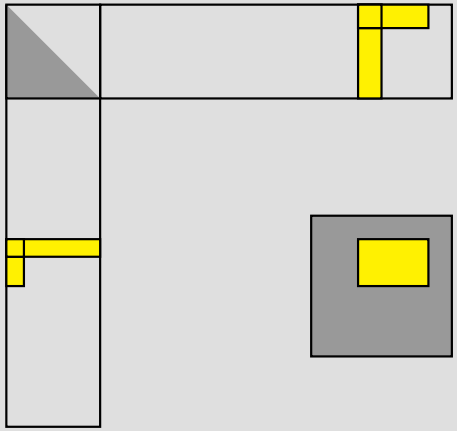
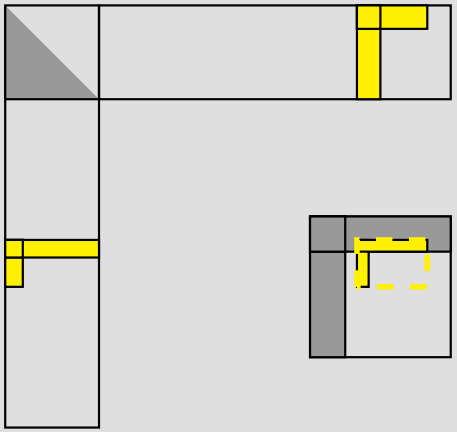


- Serie of small GEMM kernels
- Cost depends on mn

Minimal Memory



- Complex extend-add operation
- Cost depends on MN

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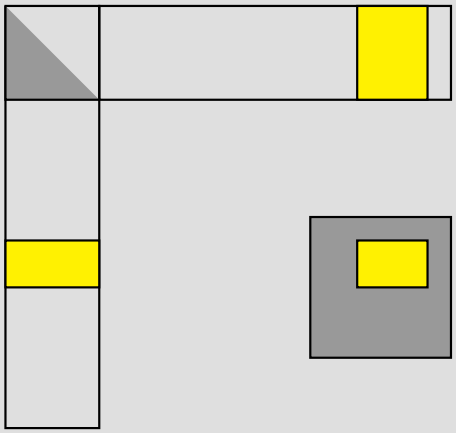

- A single GEMM kernel
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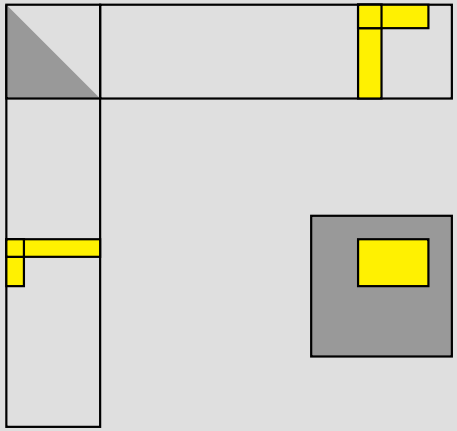
Just-In-Time



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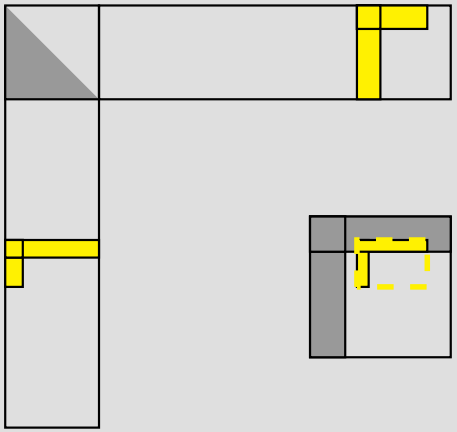
Minimal Memory



- Complex extend-add operation
- Cost depends on MN

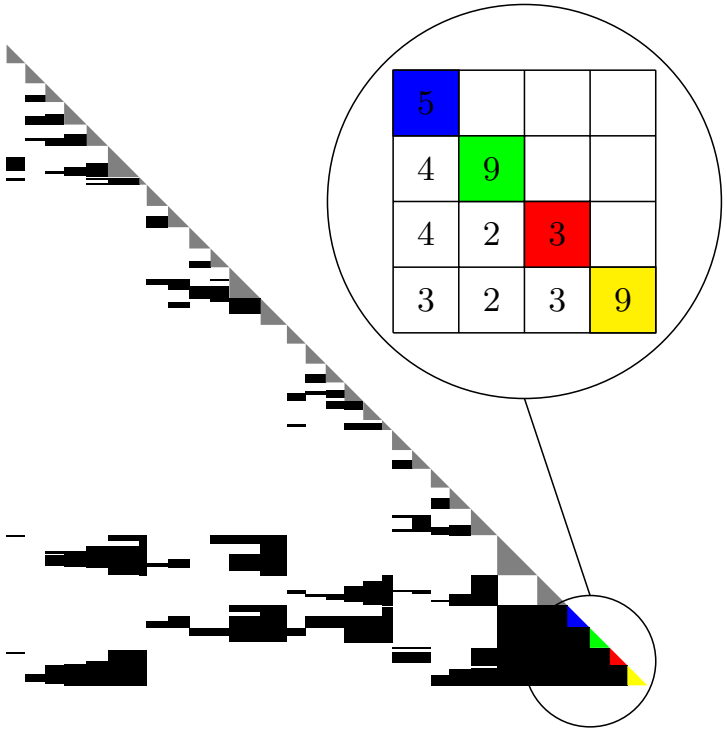
Can we reduce the number of those problematic updates?

1

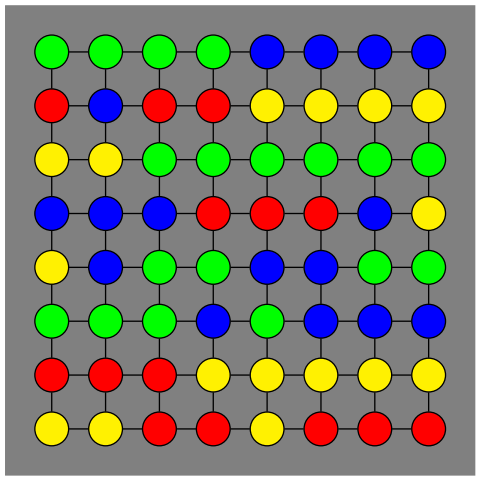
Block Low-Rank clustering techniques

Clustering techniques: existing solutions

- Supernode reordering techniques (supernodal)



(a) Symbolic factorization

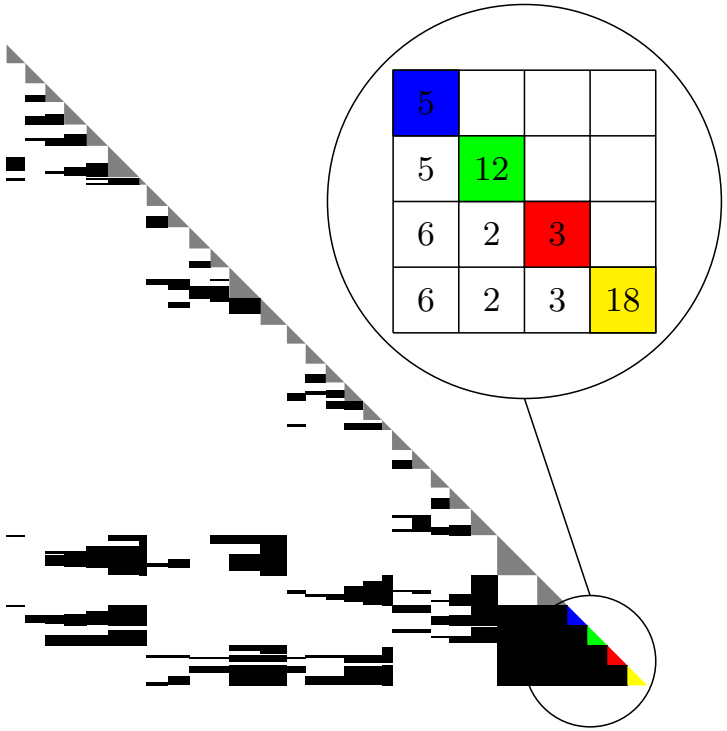


(b) First separator clustering

$8 \times 8 \times 8$ Laplacian partitioned using SCOTCH and Reordering clustering on the first separator

Clustering techniques: existing solutions

- Supernode reordering techniques (supernodal)
- k-way partitioning (dense, multifrontal)



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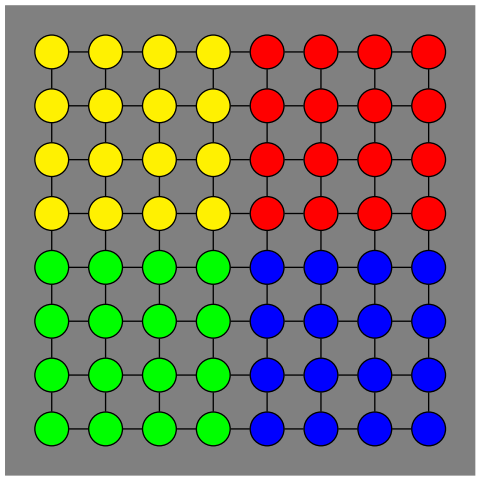


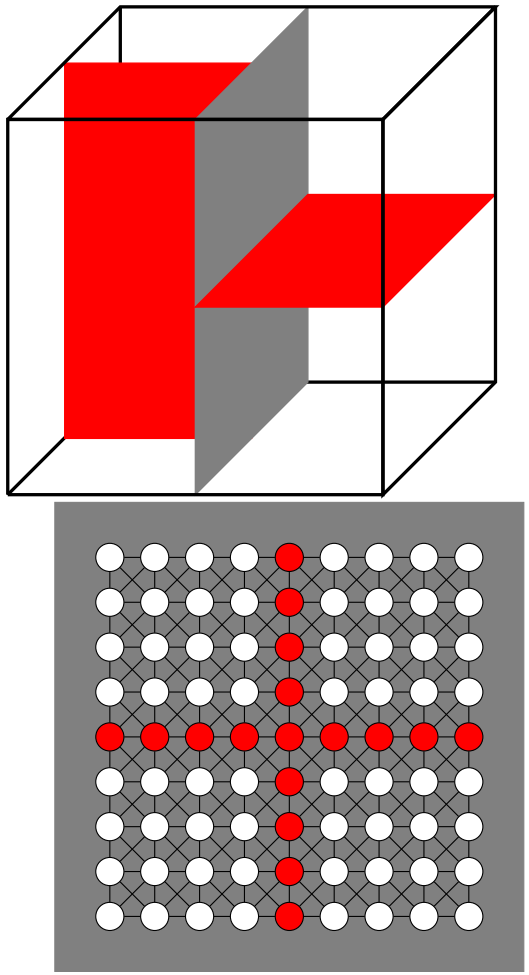
(b) First separator clustering

$8 \times 8 \times 8$ Laplacian partitioned using SCOTCH and k-way clustering on the first separator

How to take benefit from both algorithms?

Pre-selection to detect uncompressible vertices

- Pre-select unknowns that represent close interactions and will not be compressible
- Idea of Boundary Distance Low-Rank (BDLR) introduced by Darve et al.
- For instance, pre-select interactions between a father and its direct children
- Hypothesis similar to ILU(k) factorizations



How to take benefit from both algorithms?

Hierarchical Interpolative Factorization for Elliptic Operators: Differential Equations, Kenneth L. Ho and Lexing Ying, 2014.

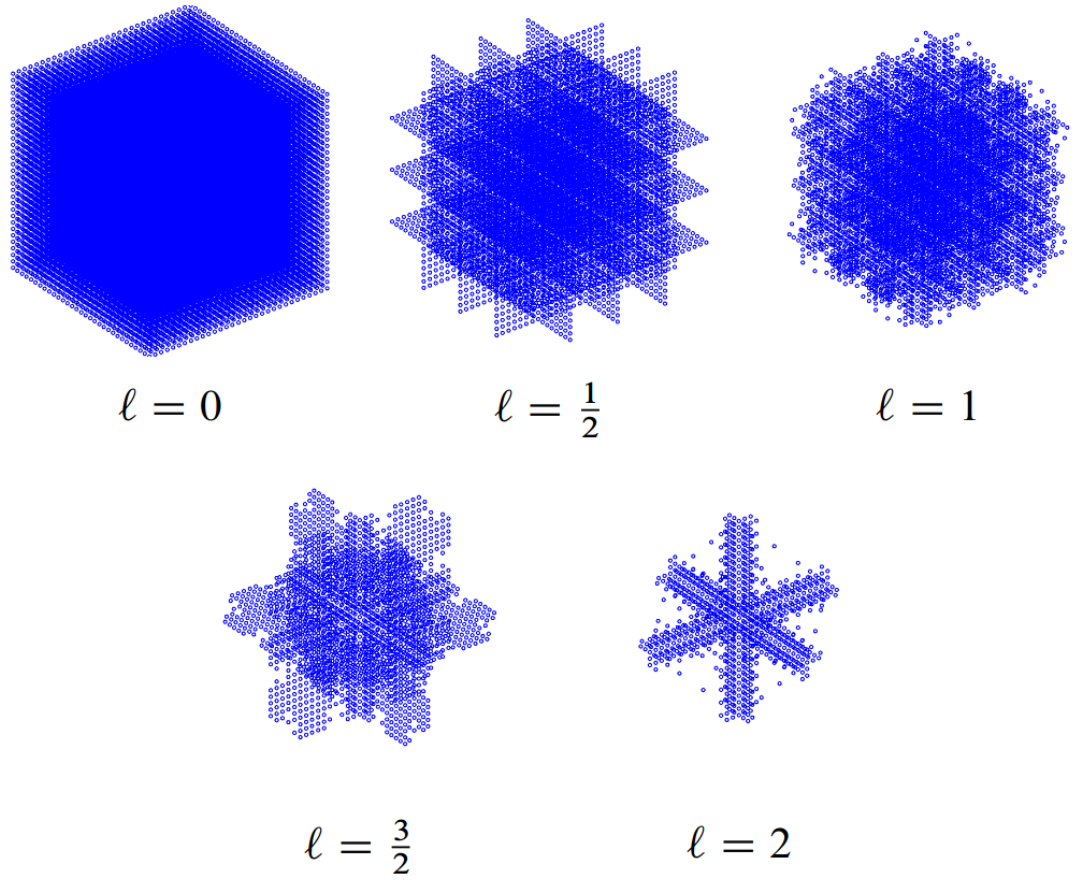


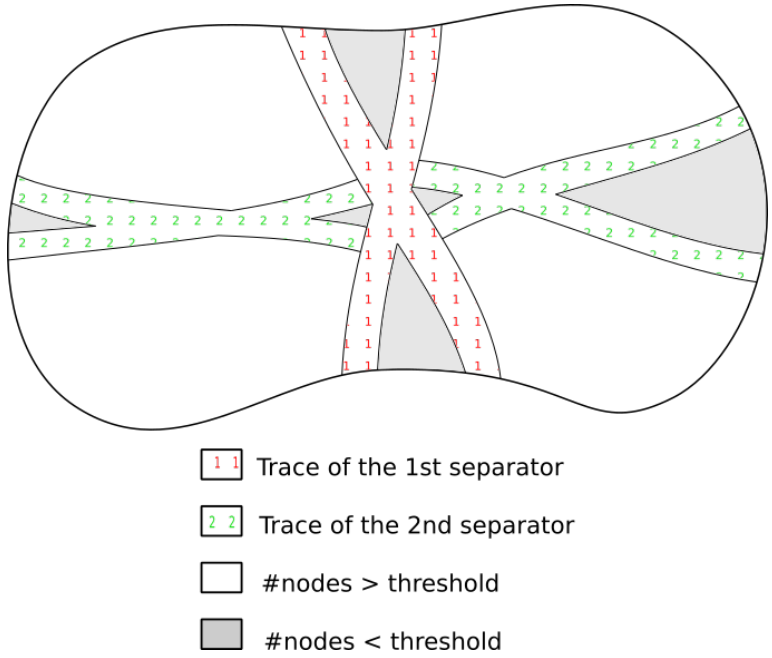
FIGURE 4.2. Active DOFs at each level ℓ of HIF-DE in 3D.

New heuristic based on projections

ComputeProjections($nblvl$, $distp$, $width$)

Lets consider a supernode and the $nblvl$ levels below in the elimination tree, with the constraint that nodes are issued from nested dissection, and not from minimum-fill as it happens at the bottom of the elimination tree.

- Each vertex of the separator being clustered is pre-selected iff it is a neighbor to one of the children at a distance $distp$
- The trace is then enlarged with neighbors within the separator at a distance $width$, similarly to BDLR.



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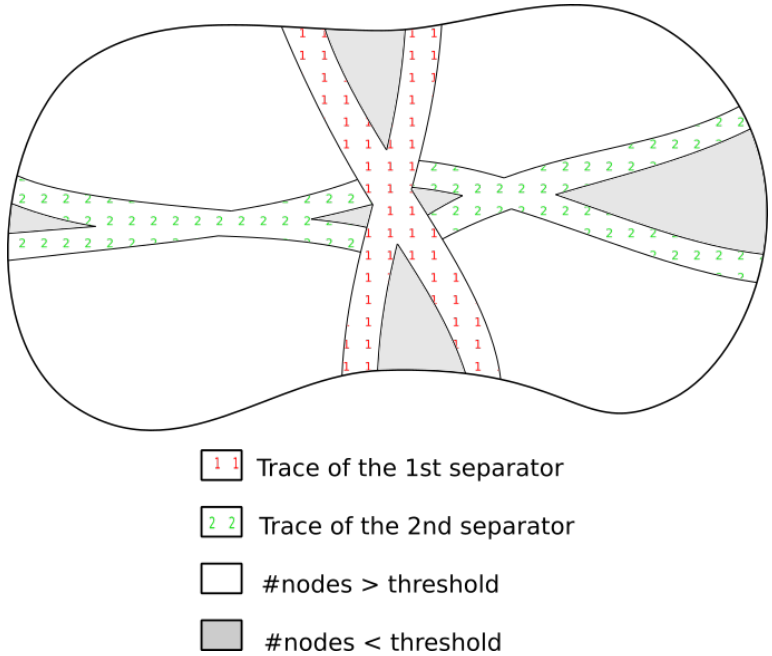
How to control the number of pre-selected vertices?

- Ensure that this number if low wrt to the total number of vertices of a separator: $\#selected < \alpha\sqrt{n}$
- Ensure that it creates at least two non-connected components



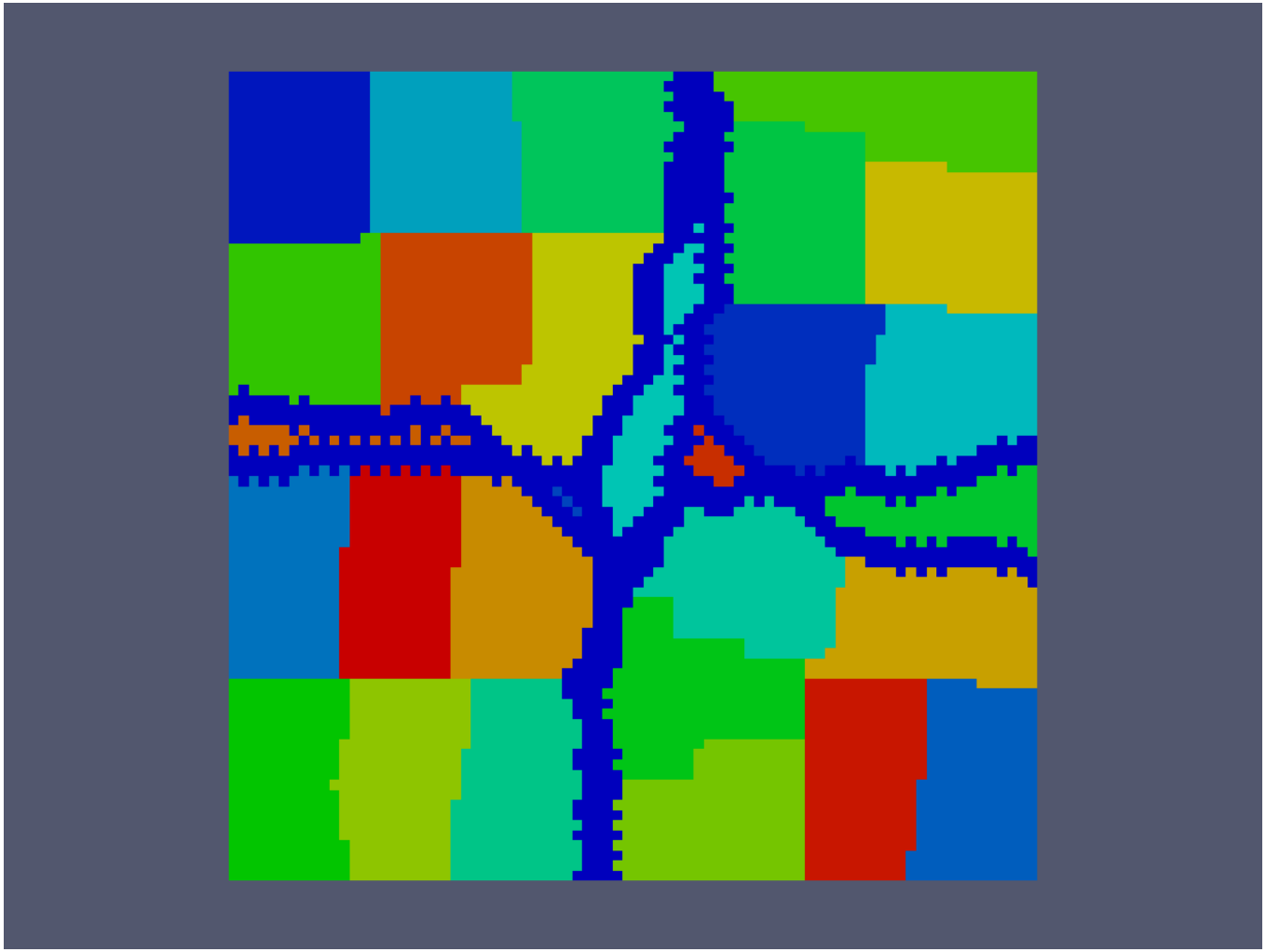
Proposed algorithm for the clustering of supernodes

Algorithm 1 Cluster a supernode

```
1: ConnectSupernode( dist )
2: ComputeProjections( levels, distp, width )
3: IsolateConnectedComponents()
4: For each connected component C Do
5:     If |C| < threshold Then
6:         Merge C into pre-selected vertices
7:     Else
8:         Kway()
9:         Reordering()
10:    End If
11: End For
12: Reordering() of pre-selected vertices
```

Projections are performed on separators of size larger than $16 \times MAX\_BLOCKSIZE$, to obtain at least four large connected subparts that will be split into four parts using kway.

Example - 80^3 Laplacian matrix



2

Numerical Experiments

Experimental setup

Architecture

- 2 INTEL Xeon $E5-2680v3$ at 2.50 GHz (24 threads)
- 128 GB

Matrices

- 33 square matrices from the SuiteSparse Matrix Collection
- real or complex
- $50K \leq N \leq 5M$
- $nb_{ops} > 1TFlops$

Solver

- PASTIX solver with SCOTCH ordering
- Static scheduling

Parameters

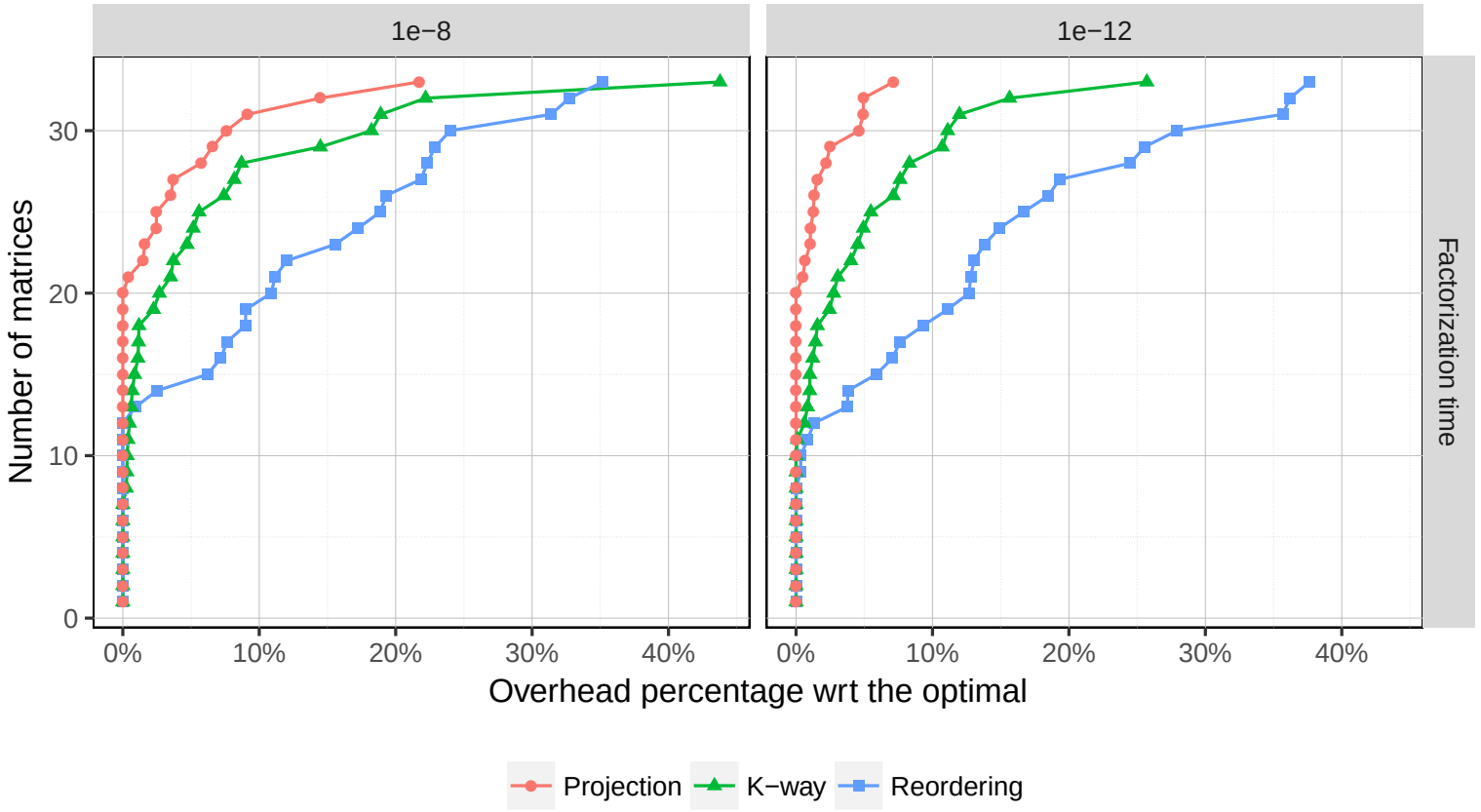
BLR solver

- Tolerance τ: absolute parameter (normalized for each block)
- Compression method is RRQR
- Compression strategy: *Minimal Memory* or *Just-In-Time*
- Blocking sizes: between 128 and 256 in following experiments

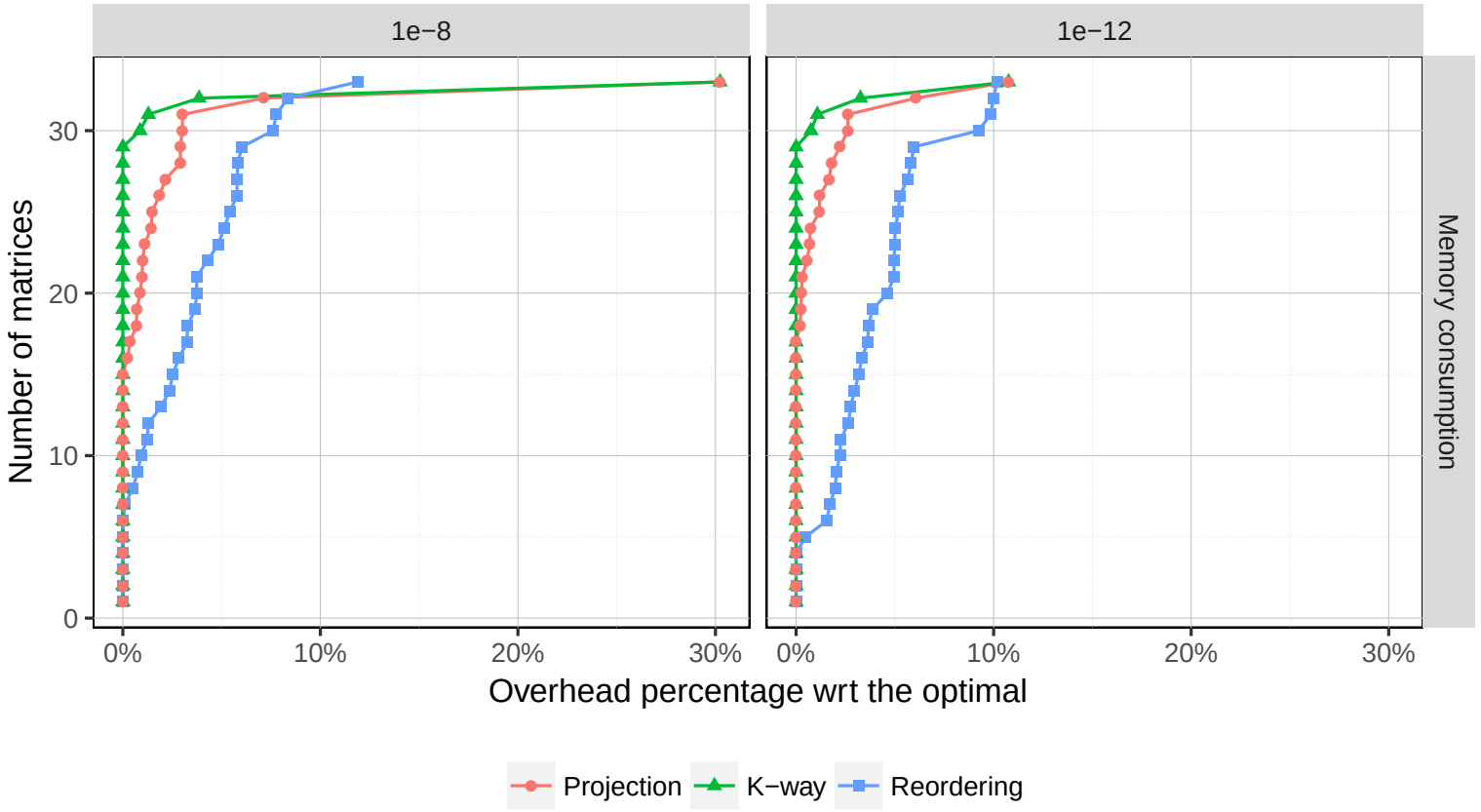
Pre-selection

- Graphs are reconnected using distance 1 in the Halo
- Selected vertices are obtained with ComputeProjections(3, 1, 1)
- Projections are performed on supernodes of size larger than 16 times the blocking size parameters.
- K-way is configured to get partition fitting the blocking size parameters
- Connected components smaller than the minimal size for low-rank compression are merged into the pre-selected vertices set.

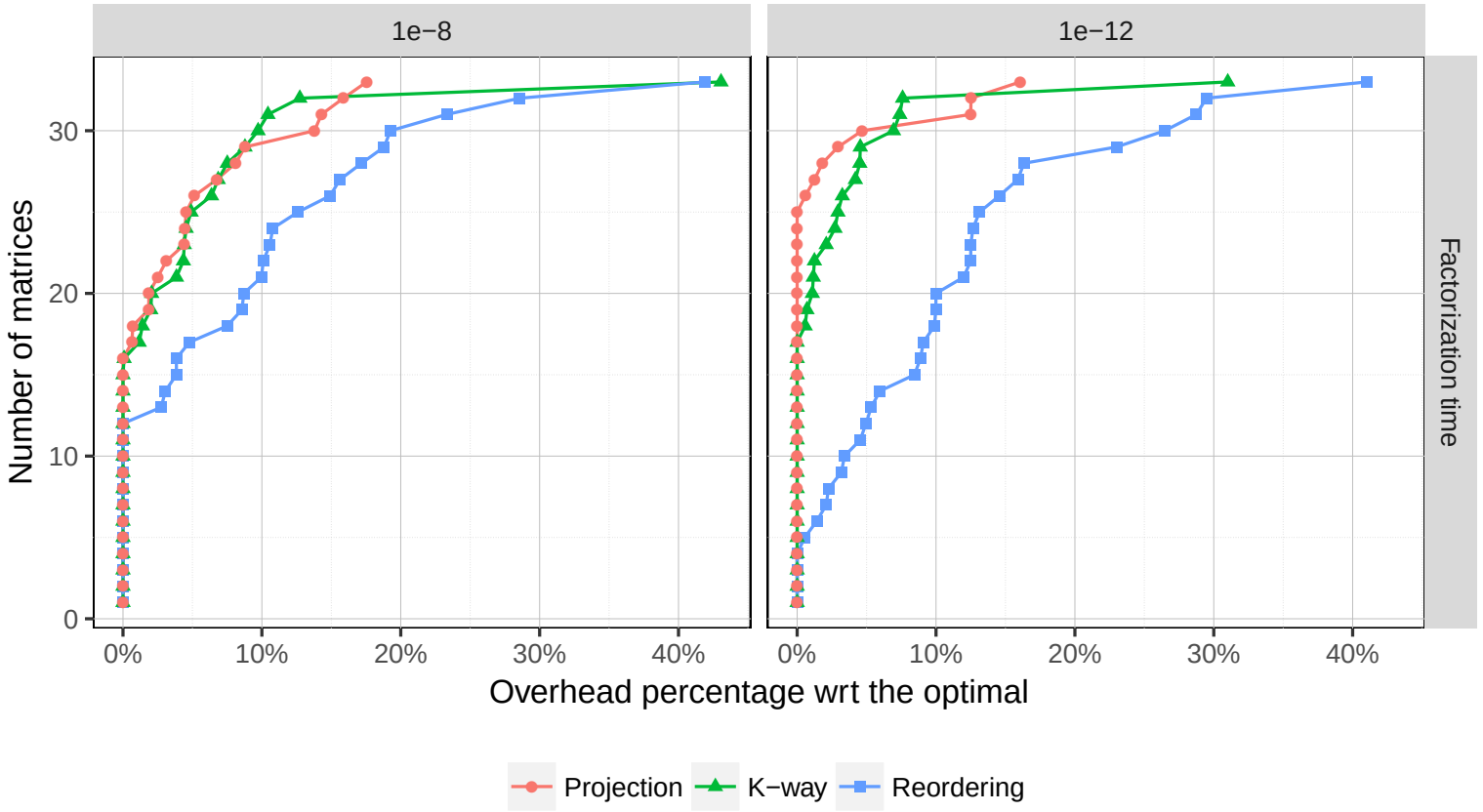
Performance profile of the factorization time – *Minimal Memory*



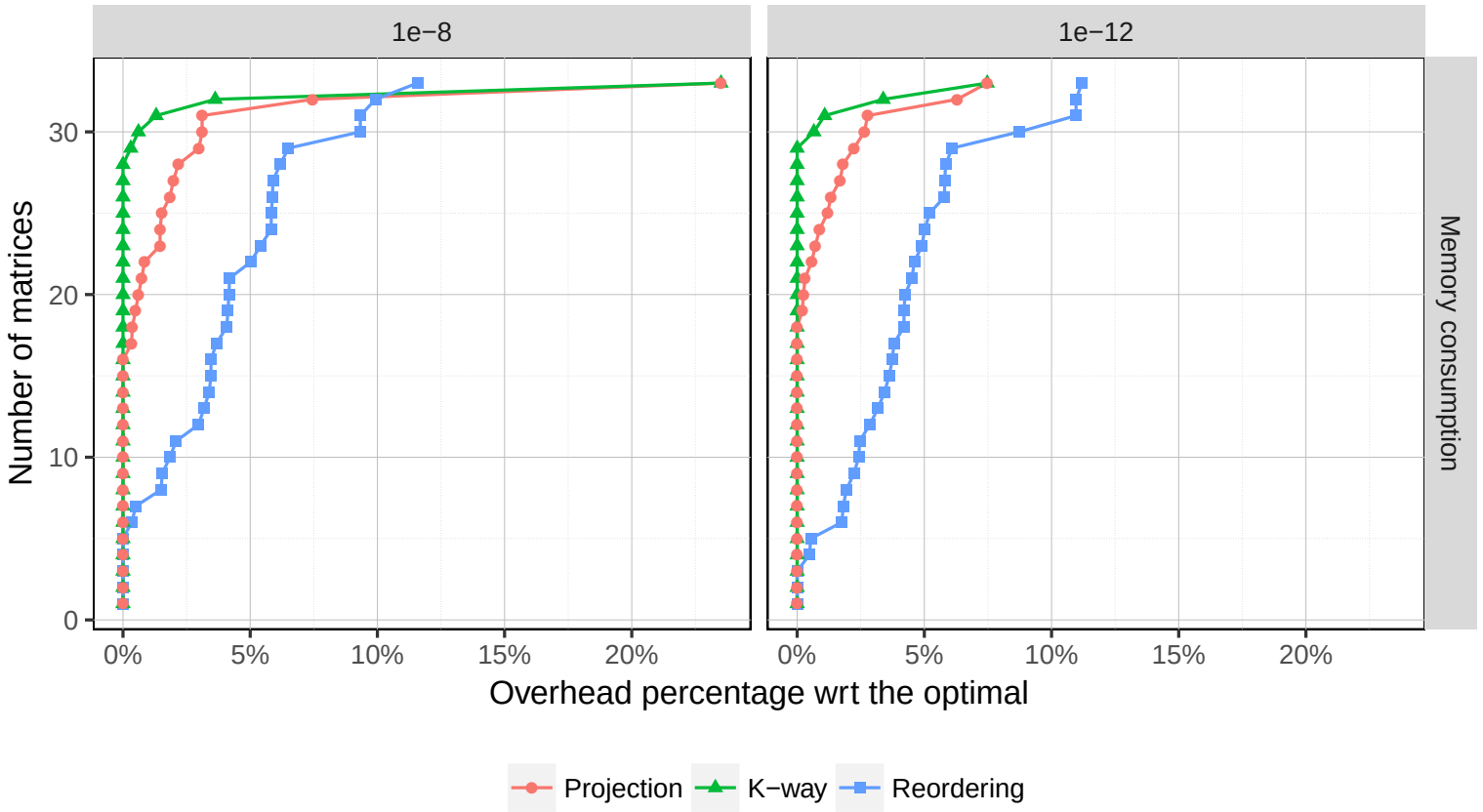
Performance profile of the memory consumption – *Minimal Memory*



Performance profile of the factorization time – *Just-In-Time*



Performance profile of the memory consumption – *Just-In-Time*



Conclusion

Ordering strategies

- Both reordering and k-way are limited to form suitable clusters
  - reordering does not allow a good compression of separators
  - k-way compresses well the separators, but does not take into account updates
- Pre-selection of some unknowns allows to obtain well-separated clusters and to exhibit non-compressible operations
- We demonstrated it is suitable for reducing time-to-solution with only a small memory consumption increase

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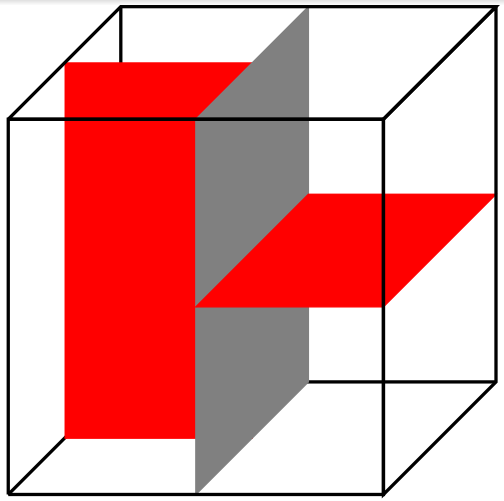
Future works

- Align separators to form clusters during the nested dissection process
- Preliminary work using fixed vertices



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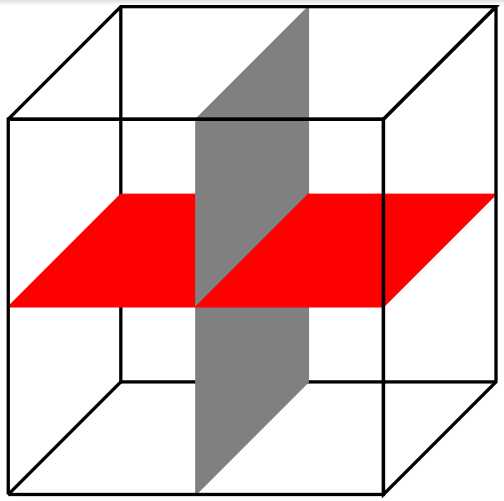

PaStiX 6.1.0

`http://gitlab.inria.fr/solverstack/pastix`

- Support shared memory with different schedulers:
  - sequential
  - static scheduler
  - PaRSEC/StarPU runtime systems with experimental GPU support
- Low-rank support
- Cholesky, LDL and LU factorizations
- GMRES, CG, BiCG iterative refinements

Thank you.